



9 December 1994

**CHEMICAL
PHYSICS
LETTERS**

Chemical Physics Letters 230 (1994) 571-579

Author index to volume 230

- Abe, K., see P. Qi 230 (1994) 322
Abou-Zied, O.K., see H.K. Sinha 230 (1994) 547
Achiba, Y., see S. Hino 230 (1994) 165
Adam, A.G., L.P. Fraser, W.D. Hamilton and M.C. Steeves, Gas-phase electronic spectroscopy of cobalt monofluoride 230 (1994) 82
Adamo, C., see F. Lelj 230 (1994) 189
Akiyama, T., see P. Qi 230 (1994) 322
Amano, T., see M. Fukushima 230 (1994) 561
Andersson, K., B.O. Roos, P.-Å. Malmqvist and P.-O. Widmark, The Cr_2 potential energy curve studied with multiconfigurational second-order perturbation theory 230 (1994) 391
Araki, S., see H. Miyasaka 230 (1994) 249
Atake, T., see K. Tanaka 230 (1994) 271
- Bache, Ø., see G. Scholz 230 (1994) 196
Baer, R., see P. Saalfrank 230 (1994) 463
Baldus, M., M. Tomaselli, B.H. Meier and R.R. Ernst, Broadband polarization-transfer experiments for rotating solids 230 (1994) 329
Balfour, W.J., see B. Simard 230 (1994) 103
Bapat, B., see K. Nagesha 230 (1994) 283
Barone, V., see F. Lelj 230 (1994) 189
Bauer, C., see A. Loettgers 230 (1994) 290
Bele, P., see R.K. Kremer 230 (1994) 255
Benkert, M. and H.-M. Vieth, Coherence transfer as a contribution to electron-nuclear cross-polarization 230 (1994) 153
Benson, J.M., see A.W. Potts 230 (1994) 543
Bhattacharyya, K., see R.K. Pathak 230 (1994) 437
Bierl, R., see S. Schneider 230 (1994) 343
Bishop, D.M. and S.M. Cybulski, Calculation of the fundamental vibrational frequencies and intensities of H_2 , D_2 , and N_2 in the presence of Li^+ or Na^+ 230 (1994) 177
Boltalina, O.V., L.N. Sidorov, E.V. Sukhanova and I.D. Sorokin, Observation of difluorinated higher fullerene anions by Knudsen cell mass spectrometry and determination of electron affinities of C_{60}F_2 and C_{70}F_2 230 (1994) 567
Borbach, M., see C.L.A. Lamont 230 (1994) 265
Borgis, D. and A. Staib, Excited states of a hydrated electron and aqueous chloride by computer simulation 230 (1994) 405
Bradshaw, A.M., see C.L.A. Lamont 230 (1994) 265
Brock, L.R., J.S. Pilgrim and M.A. Duncan, Photoionization spectroscopy of LiAl 230 (1994) 93
Brunner, H., see R.K. Kremer 230 (1994) 255

- Buenker, R.J., see J. Gu 230 (1994) 473
 Burt, S.K., see A.A. Rashin 230 (1994) 182
- Ceolín, M., M.A. Taylor and J.A. Martínez, Microscopic study of a recrystallization process from aqueous solution 230 (1994) 149
 Chakraborty, T. and E.C. Lim, Mode selective exciplex formation in photoexcited van der Waals complex of anthracene with 1,4-dimethoxybenzene 230 (1994) 137
 Chan, M.-C., see M. Fukushima 230 (1994) 561
 Chizmadzhev, Y.A., M. Maestro and F. Mavelli, A simplified kinetic model for an auto-poietic synthesis of micelles (Chem. Phys. Letters 226 (1994) 56). Erratum 230 (1994) 215
 Conrad, H., see C.L.A. Lamont 230 (1994) 265
 Cox, R.A., see O.V. Rattigan 230 (1994) 121
 Crampin, S., see P. Hu 230 (1994) 501
 Crawford, M.J., S. Haslam, J.M. Probert, Y.A. Gruzdkov and J.G. Frey, Second harmonic generation from the air/water interface of an aqueous solution of the dipeptide Boc-Trp-Trp 230 (1994) 260
 Csizmadia, I.G., see G.I. Csonka 230 (1994) 203
 Csonka, G.I., M. Loos, Á. Kucsman and I.G. Csizmadia, Ab initio study of the energy hypersurface of uneven sulfuranes. Dissociation of HCl from Cl-SH(OH)-Cl 230 (1994) 203
 Cybulski, S.M., see D.M. Bishop 230 (1994) 177
- Dang, L.X., see D.E. Smith 230 (1994) 209
 Davies, G.R., T.K. Halstead, R.C. Greenhow and K.J. Packer, High-resolution NMR of low pressure laser-polarized ^{129}Xe gas 230 (1994) 237
 Desvergne, J.-P., see D. Marquis 230 (1994) 131
 Duke, B.J., J.W. Gauld and H.F. Schaefer III, The structure of hydridogallium and hydridoaluminium bis(tetrahydroborates) 230 (1994) 306
 Duncan, M.A., see L.R. Brock 230 (1994) 93
- Engels, B., see H.U. Suter 230 (1994) 398
 Ernst, R.R., see M. Baldus 230 (1994) 329
 Ernzerhof, M., see H.U. Suter 230 (1994) 398
 Esteban, M., M. Garay, J.M. García-Tijero, E. Verdasco and A. González Ureña, Influence of the radical size on the $\text{Ca}^+ + \text{ROH} \rightarrow \text{CaOH}^+ + \text{R}$ ($\text{R} = \text{CH}_3$, C_2H_5 and C_3H_7) reaction cross section 230 (1994) 525
 Evans, I.J. and C.E. Webb, A 10 kHz pulsed tunable laser source at 308 nm for tropospheric OH detection 230 (1994) 127
- Fan, W.Y. and P.A. Hamilton, Velocity and magnetic modulation methods applied to emission spectroscopy 230 (1994) 555
 Fhadil, H.F., see A.W. Potts 230 (1994) 543
 Flores, J.R. and P. Redondo, A theoretical study of the reaction of P^+ with water. Potential energy surfaces and reaction dynamics 230 (1994) 358
 Francisco, J.S., Heat of formation determination of the ground and excited state of cyanomethylene (HCCN) radical 230 (1994) 372
 Fraser, L.P., see A.G. Adam 230 (1994) 82
 Frey, J.G., see M.J. Crawford 230 (1994) 260

- Fukushima, M., M.-C. Chan, Y. Xu, A. Taleb-Bendiab and T. Amano, High-resolution infrared absorption spectroscopy of jet-cooled molecular ions 230 (1994) 561
- Galasso, V., Theoretical study of the $^1J(^{13}\text{C}^{13}\text{C})$ indirect nuclear spin-spin coupling constant of the bridgehead bond in [1.1.1]propellane and related systems 230 (1994) 387
- Garay, M., see M. Esteban 230 (1994) 525
- García-Tijero, J.M., see M. Esteban 230 (1994) 525
- Garrison, B.J., see R.S. Taylor 230 (1994) 495
- Gauld, J.W., see B.J. Duke 230 (1994) 306
- Gausa, M., R. Kaschner, H.O. Lutz, G. Seifert and K.-H. Meiwes-Broer, Photoelectron and theoretical investigations on bismuth and antimony pentamer anions. Evidence for aromatic structure 230 (1994) 99
- Gill, P.M.W., see C.A. White 230 (1994) 8
- Gingerich, K.A., see Q. Ran 230 (1994) 337
- González Ureña, A., see M. Esteban 230 (1994) 525
- Greenhow, R.C., see G.R. Davies 230 (1994) 237
- Grimbert, D., V. Sidis and M. Sizun, Quantal characteristics of an ion-molecule complex formed by translation-to-vibration energy exchange. The $\text{H}^+ \cdots \text{O}_2$ system 230 (1994) 47
- Gruzdov, Y.A., see M.J. Crawford 230 (1994) 260
- Gu, J., G. Hirsch, R.J. Buenker, I.D. Petsalakis, G. Theodorakopoulos and M. Huang, Electronic states and radiative transitions in LiAr 230 (1994) 473
- Gu, Y., see H. Yu 230 (1994) 243
- Guha Ray, J. and P.K. Sengupta, Luminescence behavior of 7-azaindole in AOT reverse micelles 230 (1994) 75
- Hackett, P.A., see B. Simard 230 (1994) 103
- Halstead, T.K., see G.R. Davies 230 (1994) 237
- Hamilton, P.A., see W.Y. Fan 230 (1994) 555
- Hamilton, W.D., see A.G. Adam 230 (1994) 82
- Handy, N.C., see V. Termath 230 (1994) 17
- Haslam, S., see M.J. Crawford 230 (1994) 260
- Head-Gordon, M., see C.A. White 230 (1994) 8
- Heß, B.A., see U. Kaldor 230 (1994) 1
- Heully, J.-L., see P. Wind 230 (1994) 35
- Hillier, I.H., see A.W. Potts 230 (1994) 543
- Hino, S., H. Takahashi, K. Iwasaki, T. Miyazaki, K. Kikuchi and Y. Achiba, Ultraviolet photoelectron spectra of C_{78} and C_{96} 230 (1994) 165
- Hirayama, S., see A.D. Scully 230 (1994) 216
- Hirota, E., see T. Okabayashi 230 (1994) 530
- Hirsch, G., see J. Gu 230 (1994) 473
- Holovko, M.F. and E.V. Vakarin, Adsorption of the associative fluid onto the lattice of sticky sites 230 (1994) 507
- Hotop, H., see M. Movre 230 (1994) 276
- Hu, P., D.A. King, S. Crampin, M.-H. Lee and M.C. Payne, Gradient corrections in density functional theory calculations for surfaces: Co on Pd(110) 230 (1994) 501
- Hu, X.-G., Q.-S. Li and A.-C. Tang, Inelastic atom-diatom scattering in quantum phase space representation 230 (1994) 217

- Huang, M., see J. Gu 230 (1994) 473
- Irie, M., see H. Miyasaka 230 (1994) 249
- Iwasaki, K., see S. Hino 230 (1994) 165
- Jáuregui, R., see J. Récamier A. 230 (1994) 25
- Jayatilaka, D., Fourier transforms of property densities with Gaussian functions 230 (1994) 228
- Jena, P., see J. Niu 230 (1994) 299
- Jensen, V.R., see G. Scholz 230 (1994) 196
- Jeung, G.-H., Ionic and neutral characters in the singlet and triplet reaction potential surfaces of Mg-CO₂ 230 (1994) 365
- Johnson, B.G., see C.A. White 230 (1994) 8
- Jones, J.A. and A.A. Rodriguez, Oxygen and solvent intermolecular effects on the ¹³C spin-lattice relaxation process of C₆₀ in deuterated toluene at 303 K 230 (1994) 160
- Jones, R.L., see O.V. Rattigan 230 (1994) 121
- Kaldor, U. and B.A. Heß, Relativistic all-electron coupled-cluster calculations on the gold atom and gold hydride in the framework of the Douglas-Kroll transformation 230 (1994) 1
- Kanellakopulos, B., see R.K. Kremer 230 (1994) 255
- Kaschner, R., see M. Gausa 230 (1994) 99
- Khanna, S.N., see J. Niu 230 (1994) 299
- Kieninger, M., S. Suhai and I. Mayer, The chemical Hamiltonian approach in density functional theory 230 (1994) 485
- Kikas, J. and J.L. Skinner, Spectral diffusion induced by the spatial motion of point perturbors 230 (1994) 429
- Kikuchi, K., see S. Hino 230 (1994) 165
- Kim, K., see S.S. Park 230 (1994) 171
- Kim, M.S., see S.S. Park 230 (1994) 171
- King, D.A., see P. Hu 230 (1994) 501
- Kosloff, R., see P. Saalfrank 230 (1994) 463
- Kremer, R.K., B. Kanellakopulos, P. Bele, H. Brunner and F.A. Neugebauer, Weak ferromagnetism and magnetically modulated microwave absorption at low magnetic fields in 1,3,5-triphenyl-6-oxoverdazyl 230 (1994) 255
- Krishnakumar, E., see K. Nagesha 230 (1994) 283
- Kucsman, Á., see G.I. Csonka 230 (1994) 203
- Ladik, J., see J. Li 230 (1994) 414
- Lamont, C.L.A., M. Borbach, W. Stenzel, H. Conrad and A.M. Bradshaw, The adsorption and dehydrogenation of cyclohexane on the (1 × 1) and (5 × 20) surfaces of Pt{100} 230 (1994) 265
- Lawson, J.M., see M.R. Roest 230 (1994) 536
- Lee, M.-H., see P. Hu 230 (1994) 501
- Leij, F., C. Adamo and V. Barone, Role of Hartree-Fock exchange in density functional theory. Some aspects of the conformational potential energy surface of glycine in the gas phase 230 (1994) 189
- Li, J., H.-L. Liu and J. Ladik, Calculation of the electron distribution of the YBa₂Cu₃O₇ cluster using a SCF Madelung potential 230 (1994) 414
- Li, Q.-S., see X.-G. Hu 230 (1994) 217

- Li, X., see H. Yu 230 (1994) 243
- Li, X., see P. Piecuch 230 (1994) 377
- Lim, E.C., see T. Chakraborty 230 (1994) 137
- Lin, H., see Z. Wen 230 (1994) 41
- Liu, H.-L., see J. Li 230 (1994) 414
- Loettgers, A., A. Untch, M. Stumpf, R. Schinke, H.-J. Werner, C. Bauer and P. Rosmus, The Renner-Teller-induced predissociation of $\text{HCO}(\tilde{\text{A}}^2\text{A}')$. Wavepacket calculations using new ab initio potential energy surfaces 230 (1994) 290
- Loos, M., see G.I. Csonka 230 (1994) 203
- Ludwiczak, M., see H.K. Sinha 230 (1994) 547
- Lutz, H.O., see M. Gausa 230 (1994) 99
- Ma, Y., Structure determination using X-ray fluorescence interferometry 230 (1994) 451
- Maciejewski, A., see H.K. Sinha 230 (1994) 547
- Maestro, M., see Y.A. Chizmadzhew 230 (1994) 215
- Maity, D.K. and H. Mohan, Inter- and intra-molecular two-centre three-electron bonding in radical cations of alkyl bromides 230 (1994) 351
- Malmqvist, P.-Å., see K. Andersson 230 (1994) 391
- Marathe, V.R., see K. Nagesha 230 (1994) 283
- Marquis, D. and J.-P. Desvergne, A cooperative effect in sodium cation complexation by a macrocyclic bis(9,10)anthraceno-crown ether in the ground state and in the excited state 230 (1994) 131
- Martínez, J.A., see M. Ceolín 230 (1994) 149
- Marumo, S., see A. Osuka 230 (1994) 144
- Mason, E.A., see L.A. Viehland 230 (1994) 61
- Mataga, N., see A. Osuka 230 (1994) 144
- Mataga, N., see H. Miyasaka 230 (1994) 249
- Matsuzaki, Y., K. Tanaka and T. Yamabe, Static and dynamic second hyperpolarizabilities of substituted push-pull polyenes 230 (1994) 443
- Mavelli, F., see Y.A. Chizmadzhew 230 (1994) 215
- Mayer, I., see M. Kieninger 230 (1994) 485
- Meier, B.H., see M. Baldus 230 (1994) 329
- Meiwe-Broer, K.-H., see M. Gausa 230 (1994) 99
- Merz, A., see M. Movre 230 (1994) 276
- Meyer, H., Determination of alignment parameters for symmetric top molecules using non-resonant two-photon absorption 230 (1994) 510
- Meyer, H., Detection of collision-induced rotational alignment in counterpropagating beam scattering 230 (1994) 519
- Meyer, W., see M. Movre 230 (1994) 276
- Miller, M., see Q. Ran 230 (1994) 337
- Mittal, J.P., see K.I. Priyadarsini 230 (1994) 317
- Miyasaka, H., S. Araki, A. Tabata, T. Nobuto, N. Mataga and M. Irie, Picosecond laser photolysis studies on photochromic reactions of 1,2-bis(2,4,5-trimethyl-3-thienyl)maleic anhydride in solutions 230 (1994) 249
- Miyazaki, T., see S. Hino 230 (1994) 165
- Mohan, H., see K.I. Priyadarsini 230 (1994) 317
- Mohan, H., see D.K. Maity 230 (1994) 351
- Moriya, K., Creep and dc conductivity in thallium(I) nitrite crystal 230 (1994) 117

- Movre, M., W. Meyer, A. Merz, M.-W. Ruf and H. Hotop, Angle-differential electron energy spectra for the autoionization systems $\text{He}^*(2^1\text{S}) + \text{H/D}(1^2\text{S})$. Comparison between ab initio theory and experiment 230 (1994) 276
- Nagesha, K., B. Bapat, V.R. Marathe and E. Krishnakumar, The dynamics of the formation of S_2^+ from CS_2 by electron impact 230 (1994) 283
- Nestmann, B.M., see B.K. Sarpal 230 (1994) 231
- Neugebauer, F.A., see R.K. Kremer 230 (1994) 255
- Niu, J., B.K. Rao, S.N. Khanna and P. Jena, The origin of anomalous bond dissociation energies of $\text{V}^+(\text{H}_2)_n$ clusters 230 (1994) 299
- Nobuto, T., see H. Miyasaka 230 (1994) 249
- Nygren, M.A. and L.G.M. Pettersson, Theoretical modelling of metal oxides. Influence of field strength on atomic oxygen adsorption and a simple model reaction: $\text{O}_{\text{ads}} + \text{CO} \rightarrow \text{CO}_2$ 230 (1994) 456
- Okabayashi, T., M. Tanimoto, K. Tanaka and E. Hirota, Microwave spectroscopy of fluorocyanobutadiyne ($\text{F}-\text{C}=\text{C}-\text{C}=\text{C}-\text{N}$) 230 (1994) 530
- Okada, T., see A. Osuka 230 (1994) 144
- Okahara, K., see K. Tanaka 230 (1994) 271
- Okamoto, M., see A.D. Scully 230 (1994) 216
- Okazaki, K., see P. Qi 230 (1994) 322
- Ortiz, J.V., see V.G. Zakrzewski 230 (1994) 313
- Osuka, A., S. Marumo, S. Taniguchi, T. Okada and N. Mataga, Electron transfer over two porphyrins in linear porphyrin arrays 230 (1994) 144
- Pack, R.T, Conformally Euclidean internal coordinate space in the quantum three-body problem 230 (1994) 223
- Packer, K.J., see G.R. Davies 230 (1994) 237
- Paddon-Row, M.N., see M.R. Roest 230 (1994) 536
- Paldus, J., see P. Piecuch 230 (1994) 377
- Pan, Y.-K., see Y.-B. Wang 230 (1994) 480
- Park, S.S., K. Kim and M.S. Kim, Adsorption of halides on specific reaction sites on the silver sol surface as investigated by Raman spectroscopy 230 (1994) 171
- Pathak, R.K. and K. Bhattacharyya, On the nonlinear manifold energy variation method and excited state calculations 230 (1994) 437
- Payne, M.C., see P. Hu 230 (1994) 501
- Pederson, M.R., Density-functional based determination of the CH_3-CH_4 hydrogen exchange reaction barrier 230 (1994) 54
- Petsalakis, I.D., see J. Gu 230 (1994) 473
- Pettersson, L.G.M., see M.A. Nygren 230 (1994) 456
- Peyerimhoff, S.D., see B.K. Sarpal 230 (1994) 231
- Pfingst, K., see B.K. Sarpal 230 (1994) 231
- Piecuch, P., X. Li and J. Paldus, An ab initio determination of $^1\text{A}_1-^3\text{B}_1$ energy gap in CH_2 using orthogonally spin-adapted state-universal and state-specific coupled-cluster methods 230 (1994) 377
- Pilgrim, J.S., see L.R. Brock 230 (1994) 93
- Pleß, V., see H.U. Suter 230 (1994) 398
- Potts, A.W., H.F. Fhadi, J.M. Benson and I.H. Hillier, Fixed-frequency and threshold molecular photoelectron spectra of S 1s, Si 1s and Cl 1s core levels 230 (1994) 543

- Priyadarsini, K.I., H. Mohan, A.K. Tyagi and J.P. Mittal, Preparation and characterization of $\text{DABCO}^{2+}-\text{C}_{60}^{2-}$ charge transfer complex 230 (1994) 317
- Probert, J.M., see M.J. Crawford 230 (1994) 260
- Proynov, E.I., A. Vela and D.R. Salahub, Nonlocal correlation functional involving the Laplacian of the density 230 (1994) 419
- Qi, P., K. Okazaki, T. Akiyama, K. Abe and T. Shigenari, Temperature dependence of fluorescence lifetime of 2-naphthol in ice (I_h) crystal. A study of the proton motion in ice 230 (1994) 322
- Ran, Q., R.W. Schmude Jr., M. Miller and K.A. Gingerich, Mass spectrometric investigation of the thermodynamic properties of the Si_3 molecule 230 (1994) 337
- Rao, B.K., see J. Niu 230 (1994) 299
- Rashin, A.A., L. Young, I.A. Topol and S.K. Burt, Molecular dipole moments calculated with density functional theory 230 (1994) 182
- Rattigan, O.V., R.L. Jones and R.A. Cox, The visible spectrum of gaseous OBrO 230 (1994) 121
- R  camier A., J. and R. J  uregui, On the harmonic approximation to a Morse oscillator perturbed by a time-dependent interaction 230 (1994) 25
- Redondo, P., see J.R. Flores 230 (1994) 358
- Rodr  guez, A.A., see J.A. Jones 230 (1994) 160
- Roest, M.R., J.M. Lawson, M.N. Paddon-Row and J.W. Verhoeven, Identification of a totally charge separated state in completely rigid trichromophoric compounds 230 (1994) 536
- Roos, B.O., see K. Andersson 230 (1994) 391
- Rosmus, P., see A. Loettgers 230 (1994) 290
- Ruf, M.-W., see M. Movre 230 (1994) 276
- Ruhman, S., see A. Waldman 230 (1994) 110
- Saalfrank, P., R. Baer and R. Kosloff, Density matrix description of laser-induced hot electron mediated photodesorption of NO from Pt(111) 230 (1994) 463
- Salahub, D.R., see E.I. Proynov 230 (1994) 419
- Sarpal, B.K., K. Pfingst, B.M. Nestmann and S.D. Peyerimhoff, Resonances in the integral elastic scattering cross section of ozone below 20 eV 230 (1994) 231
- Sastry, G.N., see A. Waldman 230 (1994) 110
- Sato, T., see K. Tanaka 230 (1994) 271
- Schaefer III, H.F., see B.J. Duke 230 (1994) 306
- Schinke, R., see A. Loettgers 230 (1994) 290
- Schmude Jr., R.W., see Q. Ran 230 (1994) 337
- Schneider, S., R. Bierl and M. Seischab, Sub-picosecond transient grating measurements of the resonant energy transfer in cresyl violet solutions. Evidence for non-diffusive energy transport 230 (1994) 343
- Sch  ffel, K., see G. Scholz 230 (1994) 196
- Scholz, G., K. Sch  ffel, V.R. Jensen,  . Bache and M. Ystenes, Vibrational frequencies of AlF_3 . An ab initio MO study evaluating different methods on a tricky case 230 (1994) 196
- Schweiger, A., see M. Willer 230 (1994) 67
- Scully, A.D., T. Takeda, M. Okamoto and S. Hirayama, Evidence for long-range electron transfer in a diffusion-influenced bimolecular reaction from fluorescence decay measurements (Chem. Phys. Letters 228 (1994) 32). Erratum 230 (1994) 216
- Seifert, G., see M. Gausa 230 (1994) 99

- Seischab, M., see S. Schneider 230 (1994) 343
- Sengupta, P.K., see J. Guha Ray 230 (1994) 75
- Shaik, S., see A. Waldman 230 (1994) 110
- Shen, G., see H. Yu 230 (1994) 243
- Shigenari, T., see P. Qi 230 (1994) 322
- Sidis, V., see D. Grimbert 230 (1994) 47
- Sidorov, L.N., see O.V. Boltalina 230 (1994) 567
- Simard, B., P.A. Hackett and W.J. Balfour, Jet-cooled optical spectroscopy of yttrium monocarbide. Evidence for a $^4\Pi_i$ ground state 230 (1994) 103
- Sinha, H.K., O.K. Abou-Zied, M. Ludwiczak, A. Maciejewski and R.P. Steer, Origins of the differences in solvation by alkanes and perfluoroalkanes. Evidence from the S_2 - S_0 spectra of jet-cooled van der Waals complexes of xanthione and azulene 230 (1994) 547
- Sizun, M., see D. Grimbert 230 (1994) 47
- Skinner, J.L., see J. Kikas 230 (1994) 429
- Smith, D.E. and L.X. Dang, Interionic potentials of mean force for SrCl_2 in polarizable water. A computer simulation study 230 (1994) 209
- Sorokin, I.D., see O.V. Boltalina 230 (1994) 567
- Staib, A., see D. Borgis 230 (1994) 405
- Steer, R.P., see H.K. Sinha 230 (1994) 547
- Steeves, M.C., see A.G. Adam 230 (1994) 82
- Stenzel, W., see C.L.A. Lamont 230 (1994) 265
- Stumpf, M., see A. Loettgers 230 (1994) 290
- Suhai, S., see M. Kieninger 230 (1994) 485
- Sukhanova, E.V., see O.V. Boltalina 230 (1994) 567
- Sun, Q., see H. Yu 230 (1994) 243
- Suter, H.U., V. Pleß, M. Ernzerhof and B. Engels, Difficulties in the calculation of electron spin resonance parameters using density functional methods 230 (1994) 398
- Tabata, A., see H. Miyasaka 230 (1994) 249
- Tachiya, M., Energetics of electron transfer reactions in polar solvents 230 (1994) 491
- Takahashi, H., see S. Hino 230 (1994) 165
- Takeda, T., see A.D. Scully 230 (1994) 216
- Taleb-Bendiab, A., see M. Fukushima 230 (1994) 561
- Tanaka, K., T. Tanaka, T. Atake, K. Yoshizawa, K. Okahara, T. Sato and T. Yamabe, Magnetic heat capacity of TDAE-C_{60} 230 (1994) 271
- Tanaka, K., see Y. Matsuzaki 230 (1994) 443
- Tanaka, K., see T. Okabayashi 230 (1994) 530
- Tanaka, T., see K. Tanaka 230 (1994) 271
- Tang, A.-C., see X.-G. Hu 230 (1994) 217
- Taniguchi, S., see A. Osuka 230 (1994) 144
- Tanimoto, M., see T. Okabayashi 230 (1994) 530
- Tao, F.-M., see Y.-B. Wang 230 (1994) 480
- Taylor, M.A., see M. Ceolin 230 (1994) 149
- Taylor, R.S. and B.J. Garrison, Molecular dynamics simulations of keV particle bombardment. Correlation of intact molecular ejection with adsorbate size 230 (1994) 495
- Terazima, M., Transient lens spectroscopy in a fast time scale. Photoexcitation of rhodamine 6G and methyl red solution 230 (1994) 87

- Termath, V. and N.C. Handy, A Kohn-Sham method involving the direct determination of the Coulomb potential on a numerical grid 230 (1994) 17
- Theodorakopoulos, G., see J. Gu 230 (1994) 473
- Tomaselli, M., see M. Baldus 230 (1994) 329
- Topol, I.A., see A.A. Rashin 230 (1994) 182
- Tyagi, A.K., see K.I. Priyadarsini 230 (1994) 317
- Untch, A., see A. Loettgers 230 (1994) 290
- Vakarin, E.V., see M.F. Holovko 230 (1994) 507
- Vela, A., see E.I. Proynov 230 (1994) 419
- Verdasco, E., see M. Esteban 230 (1994) 525
- Verhoeven, J.W., see M.R. Roest 230 (1994) 536
- Viehland, L.A. and E.A. Mason, Long-range interaction of protons and deuterons with neon atoms 230 (1994) 61
- Vieth, H.-M., see M. Benkert 230 (1994) 153
- Waldman, A., S. Ruhman, S. Shaik and G.N. Sastry, Coherent photochemistry in solution. Impulsive photoselective photolysis of $Mn_2(CO)_{10}$ 230 (1994) 110
- Wang, L., see H. Yu 230 (1994) 243
- Wang, Y., see Z. Wen 230 (1994) 41
- Wang, Y.-B., F.-M. Tao and Y.-K. Pan, $H_2S \cdots HOH$ or $H_2O \cdots HSH$, which is more stable in the water-hydrogen sulfide complex? 230 (1994) 480
- Webb, C.E., see I.J. Evans 230 (1994) 127
- Wen, Z., Y. Wang and H. Lin, Explicit formulae for spin-dependent matrix elements in the unitary group approach 230 (1994) 41
- Werner, H.-J., see A. Loettgers 230 (1994) 290
- White, C.A., B.G. Johnson, P.M.W. Gill and M. Head-Gordon, The continuous fast multipole method 230 (1994) 8
- Widmark, P.-O., see K. Andersson 230 (1994) 391
- Willer, M. and A. Schweiger, Forbidden-transition-labelled EPR (FORTE). An approach for the sensitive measurement of forbidden EPR transitions 230 (1994) 67
- Wind, P. and J.-L. Heully, Reduction of the basis set superposition error at the correlation level 230 (1994) 35
- Xu, Y., see M. Fukushima 230 (1994) 561
- Yamabe, T., see K. Tanaka 230 (1994) 271
- Yamabe, T., see Y. Matsuzaki 230 (1994) 443
- Yin, Y., see H. Yu 230 (1994) 243
- Yoshizawa, K., see K. Tanaka 230 (1994) 271
- Young, L., see A.A. Rashin 230 (1994) 182
- Ystenes, M., see G. Scholz 230 (1994) 196
- Yu, H., Y. Gu, Q. Sun, Y. Yin, X. Li, G. Shen and L. Wang, Dissociative excitation of CH_3NO_2 and CH_3OH by collisions with metastable helium in the beam experiment 230 (1994) 243
- Zakrzewski, V.G. and J.V. Ortiz, Vertical ionization energies of cubane 230 (1994) 313